Modern Code Validation: How Do We Do It?

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Outline

- Traditional experiments vs. validation experiments
  - Validation hierarchy
  - Existing validation databases
- Characteristics of a validation experiment
- Nondeterministic simulation of experiments
  - Experimental uncertainties
  - Model form uncertainty
- Suggestions for the path forward

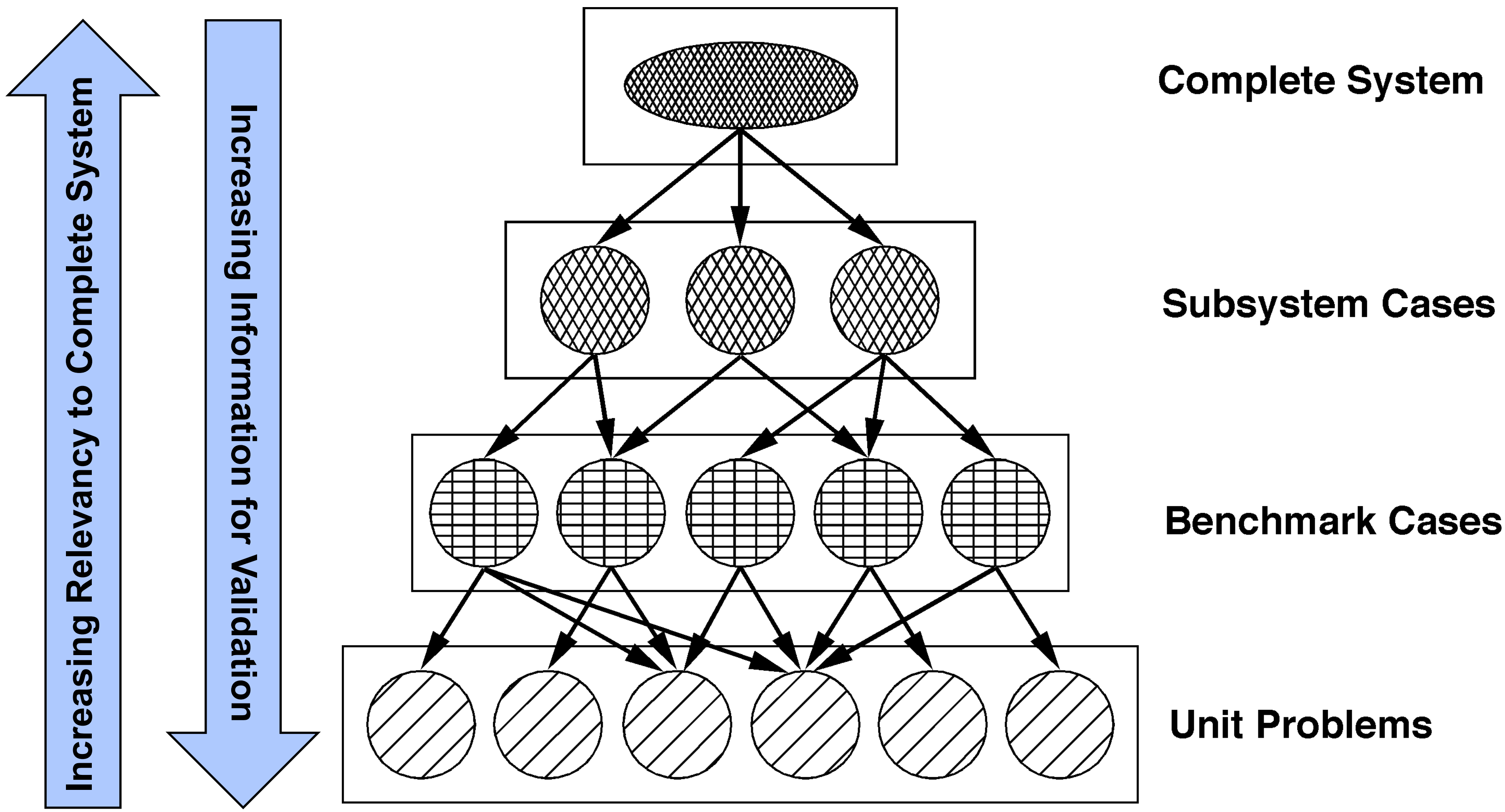
Traditional Experiments vs. Validation Experiments

Goals of traditional experiments:

1. **Improve the fundamental understanding of the physics:**
   - **Ex: performance of new fuels; departure from nucleate boiling**
2. **Determine parameters in existing mathematical models:**
   - **Ex: model calibration experiment for bubbly flows; model calibration experiment for crack propagation in fuels**
3. **Assess subsystem or complete system performance:**
   - **Ex: loss of coolant experiment; plant safety performance during various subsystem failure and excitation scenarios**

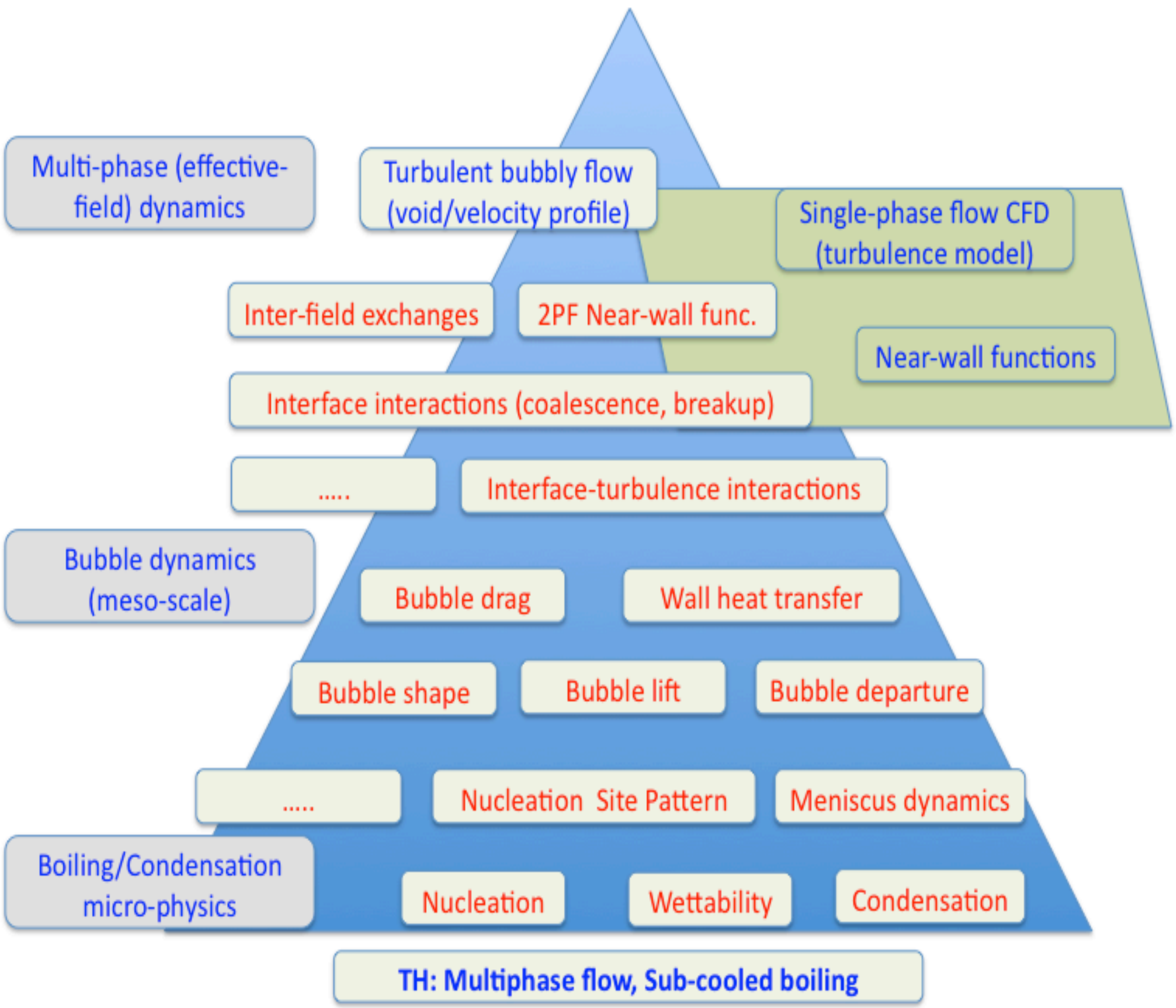
- **Goal of a model validation experiment:**
  - **An experiment that is designed and executed to quantitatively estimate a mathematical model's ability to simulate a well characterized experiment.**
- **The customer of a model validation experiment is usually a model developer or computational analyst.**

Validation Experiment Hierarchy



(Ref: AIAA Guide, 1998)

Validation Hierarchy for Sub-cooled Boiling



A validation hierarchy can be constructed at any level of physical process

(Ref: Dinh, 2012)

Examples of Validation Databases Related to Nuclear Power

- Organization for Economic Co-operation and Development/ Nuclear Energy Agency (OECD/NEA), International Fuel Performance Experiments (IFPE) Database
- OECD/NEA Shielding Integral Benchmark Archive and Database (SINBAD)
- OECD/NEA International Reactor Physics Benchmark Experiment Evaluation (IRPhE) Project
- OECD/NEA Expert Group on Multi-Physics Experimental Data, Benchmark, and Validation (EGMPEBV), newly formed
- Generation IV Materials Handbook database
- Loss-of-Fluid Test (LOFT) database at INL
- Proprietary or classified databases, e.g., Westinghouse Advanced Loop Testing, Bettis Atomic Power Laboratory, Knolls Atomic Power Laboratory, etc.

Six Characteristics of a Validation Experiment

1. A validation experiment should be jointly designed and executed by experimentalists and computationalists:
   – Close working relationship from inception to documentation
   – Elimination of the typical competition between each
   – Complete candor concerning strengths and weaknesses
2. A validation experiment should be designed to capture the relevant physics, all initial and boundary conditions, and all auxiliary data needed for a simulation:
   – Computational simulation input data should be measured in the experiment and key modeling assumptions understood
   – Characteristics and imperfections of the experimental facility should be measured and included in the simulation

(Ref: Aeschliman and Oberkampf, 1998)

Characteristics of a Validation Experiment (continued)

3. A validation experiment should use any possible synergisms between experiment and computational approaches:
   - Offset strengths and weaknesses of computation and experiment
   - Use simulations of the “empty” facility to better understand the operation of the facility
   - Use experimental data from the “empty” facility to calibrate certain model parameters

4. Independence between computational and experimental results should be maintained where possible:
   - The flavor of a blind comparison should be maintained if possible
   - All input data needed for the simulation should be measured and provided
   - Once system response measurements are available to the analyst, calibration usually occurs

Characteristics of a Validation Experiment (continued)

5. A hierarchy of experimental measurements should be made which presents an increasing range of computational difficulty:
   - Qualitative data (e.g., visualization) and quantitative data
   - Functionals, local variables, derivatives of local variables
   - Computational solution data should be processed in a manner similar to the experimental measurement data
6. Carefully employ experimental uncertainty analysis procedures to delineate and quantify random and correlated bias errors:
   - Experimentalist should provide uncertainty estimates on system response data and input quantities needed by the code
   - Use traditional or statistical design of experiments methods to estimate random and correlated bias errors in measurements
   - If possible, conduct experiments using different diagnostic techniques or different experimental facilities

What is the Goal of a Model Validation Experiment?

- Estimation of the model form uncertainty for the specific conditions and physics of the experiment
- What makes this difficult?
  - Measurement of all important model input data
  - Estimation of response variability and measurement uncertainty
- Measured input data characterizes:
  - System geometry
  - Initial conditions
  - System physical parameters
  - Boundary conditions
  - System excitation
- As a result, the experimentalist must:
  - Measure and document model input and system response data
  - Estimate and document experimental uncertainty on both model input data and system response data

Nondeterministic Simulation of Experiments

- **Computational simulation can be viewed as a mapping of input data to output data using the mathematical model**

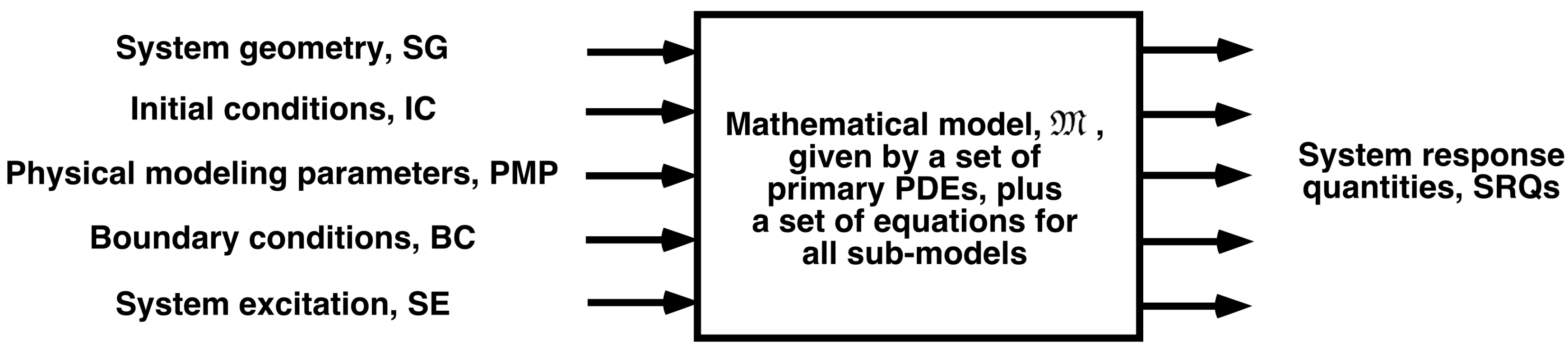
$$\mathfrak{M}(SG, IC, PMP, BC, SE) \rightarrow SRQ$$

- **Because of missing data or variability of input data from the experiment, we must conduct non-deterministic simulations**

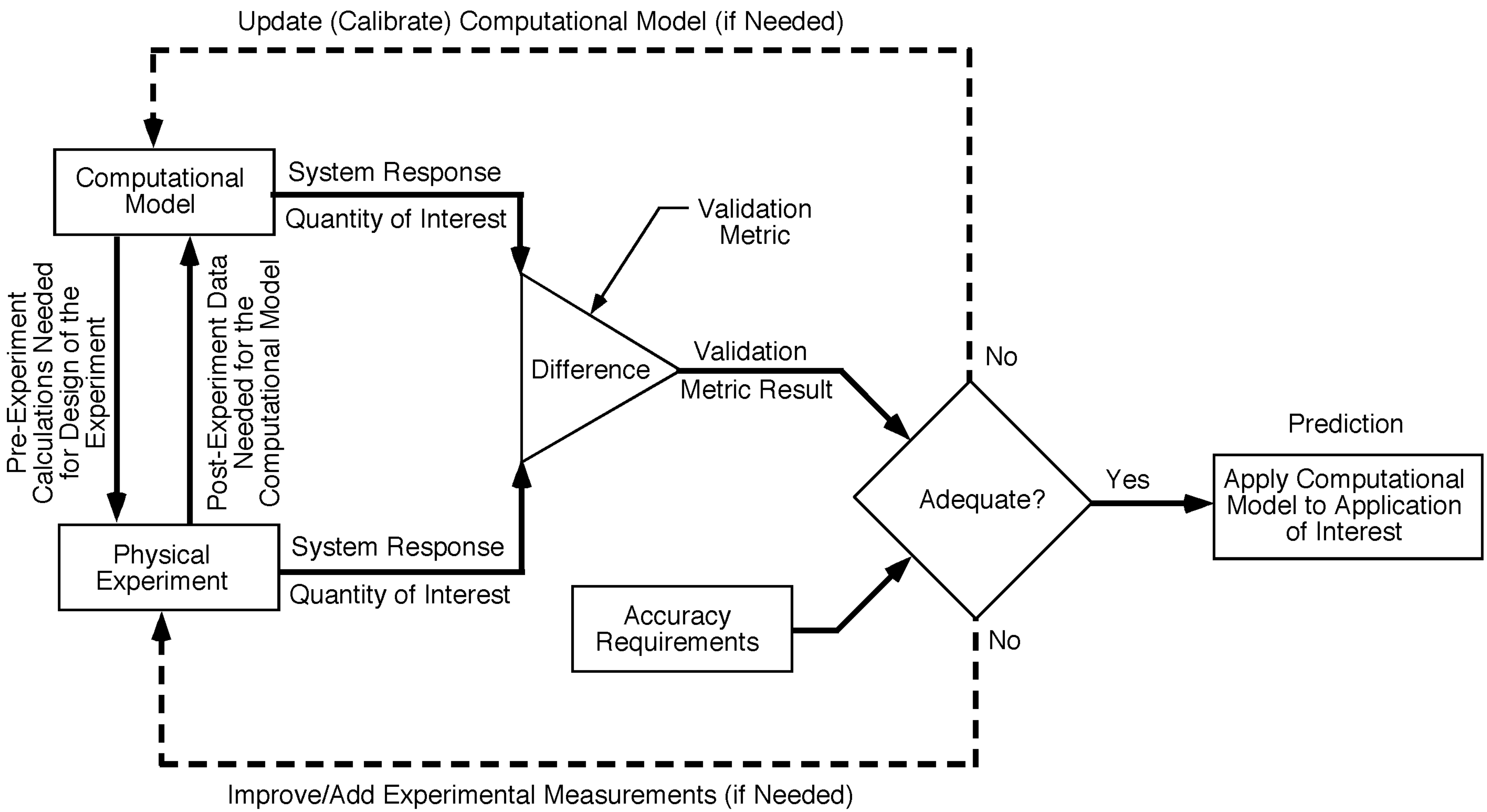
Uncertain inputs to the model

Propagation of uncertainties through the model

Uncertain outputs from the model



Model Accuracy Assessment, Calibration and Prediction

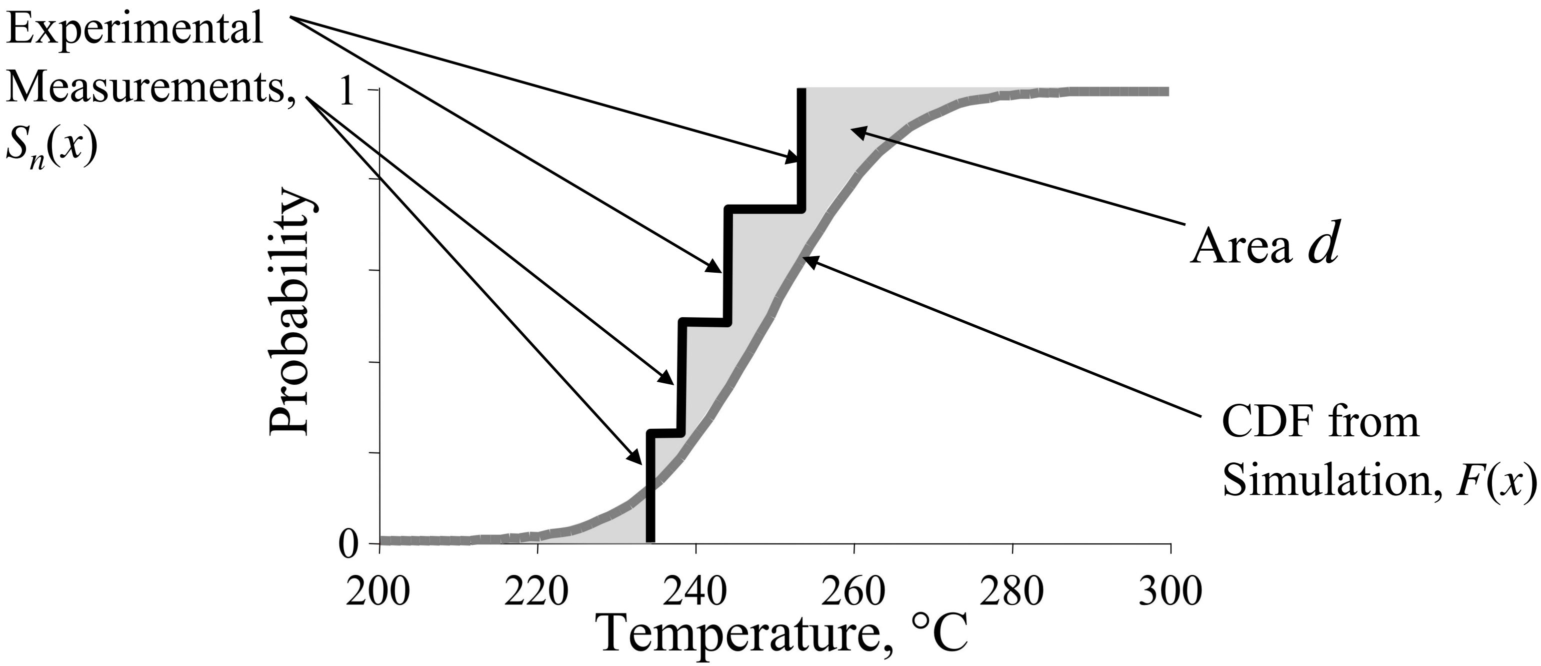


(from Oberkampf and Barone, 2006)

Example of a Validation Metric: Area Metric

- **The validation metric is defined to be the area between the CDF from the simulation and the empirical distribution function (EDF) from the experiment**

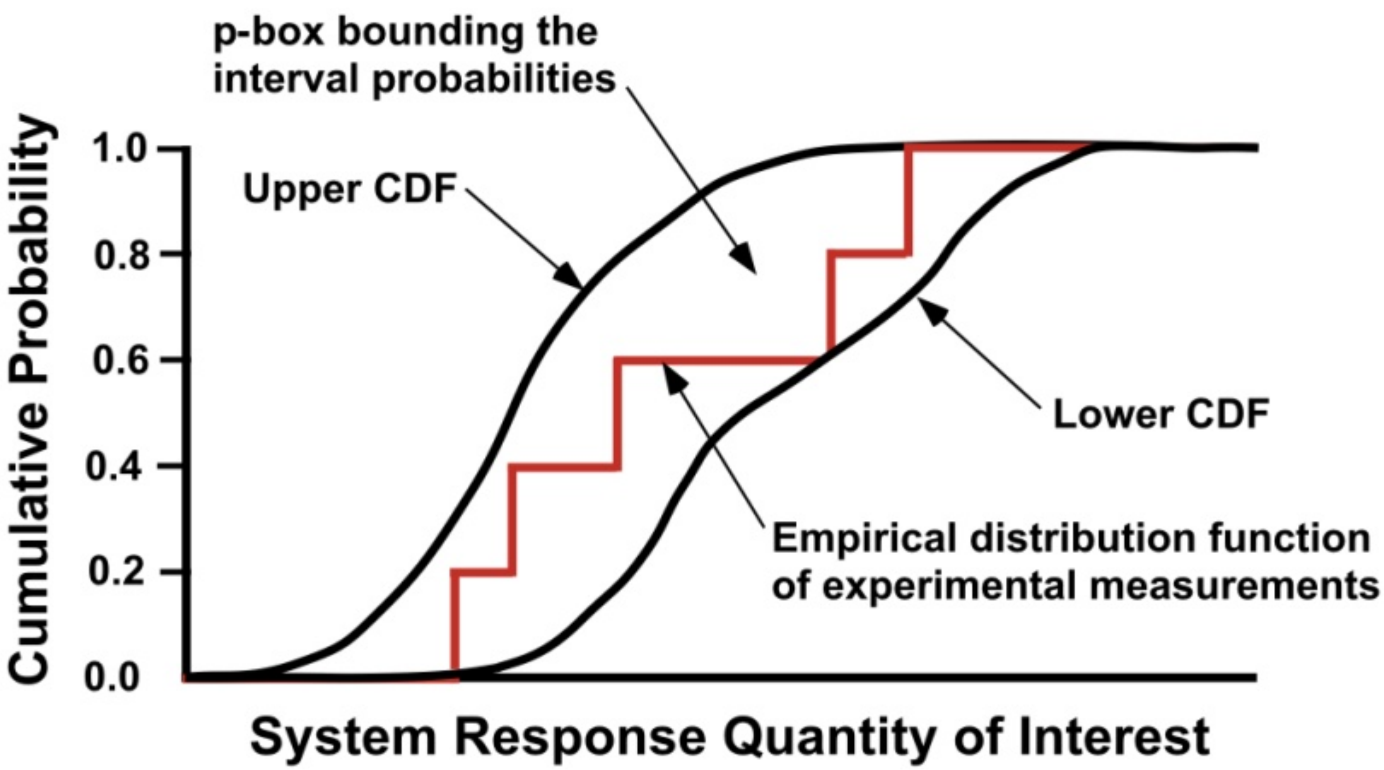
$$d(F, S_n) = \int_{-\infty}^{\infty} \left| F(x) - S_n(x) \right| \mathrm{d}x \qquad \text{(Minkowski } L_1 \text{ metric)}$$



(Ref: Ferson et al, 2008)

What is the Impact of Missing Input Data from the Experiment?

- **Unmeasured or undocumented input data leads to <u>either</u>:**
  - **Calibration or tuning of parameters in the model**
  - **Increased uncertainty in the predicted output. This does <u>not</u> allow us to critically assess the predictive accuracy of the model.**



(Ref: Oberkampf and Roy, 2010)

Suggestions for the Path Forward

- **Evaluation of existing experimental databases for completeness and documentation of:**
  - **Input data needed for simulation**
  - **Estimation of experimental uncertainty on both input and output data**
  - **Existence of multiple experimental realizations or different facilities**
- **Which perspective is more constructive for planning new validation experiments?**

Physical processes in need of improved modeling **versus** ***Applications areas in need of improved understanding***

- **Whichever perspective is used, conduct simulations of planned experiments to determine the most important <u>input data</u> to be measured, i.e., conduct sensitivity analyses**
- **Improve the understanding of recommended characteristics of validation experiments among experimentalists and analysts**

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